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ABSTRACT: The path decomposition expansion is a path integral technique for decomposing sums over paths in configuration space into sums over paths in different spatial regions. It leads to a decomposition of the configuration space propagator across arbitrary surfaces in configuration space. It may be used, for example, in calculations of the distribution of first crossing times. The original proof relied heavily on the position representation and in particular on the properties of path integrals. In this paper, an elementary proof of the path decomposition expansion is given using projection operators. This leads to a version of the path decomposition expansion more general than the configuration space form previously given. The path decomposition expansion in momentum space is given as an example.

The propagator in non-relativistic quantum mechanics is commonly represented by a sum over paths:

$$g(\mathbf{x}'', t'' | \mathbf{x}', t') \equiv \langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t'' - t')} | \mathbf{x}' \rangle \quad (1.1)$$

$$= \int \mathcal{D}\mathbf{x}(t) \exp \left( \frac{i}{\hbar} S[\mathbf{x}(t)] \right) \quad (1.2)$$

Here, as usual,  $S[\mathbf{x}(t)]$  is the action and the sum is over paths  $\mathbf{x}(t)$  in a  $d$ -dimensional configuration space satisfying the boundary conditions  $\mathbf{x}(t') = \mathbf{x}'$ ,  $\mathbf{x}(t'') = \mathbf{x}''$ . The paths in Eq.(1.2) move *forwards* in time. An important consequence of this feature is the composition property of the propagator: Consider an intermediate surface labeled by  $t$ , so  $t' < t < t''$ . Then because the paths move forwards in time, they intersect the surface labeled by  $t$  once and only once, at a point  $\mathbf{x}$ , say. The paths summed over may therefore be partitioned according to the value  $\mathbf{x}$  at which they cross the surface labeled by  $t$ , and one readily derives the composition law [1,2],

$$g(\mathbf{x}'', t'' | \mathbf{x}', t') = \int d^d \mathbf{x} g(\mathbf{x}'', t'' | \mathbf{x}, t) g(\mathbf{x}, t | \mathbf{x}', t') \quad (1.3)$$

A more complicated story arises in the case of decomposition of the propagator across general surfaces in configuration space. The paths  $\mathbf{x}(t)$  in configuration space go backwards and forwards in each of the coordinates  $x_1, x_2, \dots$ , and will generally cross a given surface  $\Sigma$ , such as  $x_1 = \text{constant}$ , many times. The point of crossing is therefore not well-defined. However, what is well-defined is the time and location of *first* crossing of a surface  $\Sigma$ . That is, the paths connecting  $\mathbf{x}'$  at time  $t'$  to  $\mathbf{x}''$  at time  $t''$  (where  $\mathbf{x}'$  and  $\mathbf{x}''$  lie on opposite sides of a surface  $\Sigma$ ) may be partitioned according to the time  $t_\sigma$  and location  $\mathbf{x}_\sigma$  of first crossing. Corresponding to this partition of the paths is a decomposition of the propagator called the path decomposition expansion, or PDX [2,3,4,5],

$$g(\mathbf{x}'', t'' | \mathbf{x}', t') = \int_{t'}^{t''} dt_\sigma \int_\Sigma d^{d-1} \mathbf{x} g(\mathbf{x}'', t'' | \mathbf{x}_\sigma, t_\sigma) \frac{i\hbar}{2m} \mathbf{n} \cdot \nabla g^{(r)}(\mathbf{x}_\sigma, t_\sigma | \mathbf{x}', t') \quad (1.4)$$

Here,  $g^{(r)}$  is the restricted propagator on the side of  $\Sigma$  containing  $\mathbf{x}'$ , and  $\mathbf{n}$  is the normal to the surface  $\Sigma$  pointing away from the region of restricted propagation. The restricted

propagator  $g^{(r)}$  is defined to vanish on  $\Sigma$  but its normal derivative does not. Eq.(1.4) consists of two parts. The first term in the integrand describes unrestricted propagation from the surface to the final point. The second term therefore describes the sum over paths which never cross  $\Sigma$  but end on it at  $\mathbf{x}_\sigma$  at time  $t_\sigma$ . One may also consider the case in which the initial and final points lie on the same side of  $\Sigma$ , which leads to the expression,

$$g(\mathbf{x}'', t'' | \mathbf{x}', t') = g^{(r)}(\mathbf{x}'', t'' | \mathbf{x}', t') + \int_{t'}^{t''} dt_\sigma \int_\Sigma d^{d-1}\mathbf{x} g(\mathbf{x}'', t'' | \mathbf{x}_\sigma, t_\sigma) \frac{i\hbar}{2m} \mathbf{n} \cdot \nabla g^{(r)}(\mathbf{x}_\sigma, t_\sigma | \mathbf{x}', t') \quad (1.5)$$

where again the normal  $\mathbf{n}$  points away from the region of restricted propagation.

The PDX was originally introduced in connection with calculations concerning tunneling [3]. It has since been used to derive the composition laws of relativistic quantum mechanics from their path integral representation [2]. It is clearly also of use for computing spacetime coarse grainings in non-relativistic quantum mechanics, *i.e.*, probabilities of certain types of alternatives which cannot be expressed in terms of a wave function at a single moment of time [6,7].

An example of a spacetime coarse graining in which the above formulae are useful is the first crossing time distribution. The amplitude to start in a state  $\Psi(\mathbf{x}', t')$  with support on one side of  $\Sigma$  only, to cross the surface for the first time  $\Sigma$  in the time interval  $[t_1, t_2]$  (where  $t' < t_1 < t_2 < t''$ ), and then to end up at  $\mathbf{x}''$  at time  $t''$ . This is given by

$$A(t_1, t_2, \mathbf{x}'', t'') = \int d^d\mathbf{x}' \int_{t_1}^{t_2} dt_\sigma \int_\Sigma d^{d-1}\mathbf{x} g(\mathbf{x}'', t'' | \mathbf{x}_\sigma, t_\sigma) \times \frac{i\hbar}{2m} \mathbf{n} \cdot \nabla g^{(r)}(\mathbf{x}_\sigma, t_\sigma | \mathbf{x}', t') \Psi(\mathbf{x}', t') \quad (1.6)$$

The candidate probability of crossing the surface for the first time in the time interval  $[t_1, t_2]$  is therefore

$$p(t_1, t_2) = \int d^d\mathbf{x}'' |A(t_1, t_2, \mathbf{x}'', t'')|^2 \quad (1.7)$$

It is referred to as a candidate probability because the so-called “probability sum rules” are not in general satisfied by objects constructed in this way, and thus (1.7) is not a true probability. In this case, the rule to be satisfied is that the candidate probability (1.7)

and the probability of never crossing the surface in the time interval  $[t_1, t_2]$  must sum to 1. This is generally not true unless the initial state is restricted in some way, or the system is coupled to a wider environment [6,7]. We will not go into this issue here, although it is often important to keep it in mind.

The original proof of the PDX involved a detailed treatment of the Euclidean path integral, and relied on a particular integral identity [3]. A more sophisticated proof was given in Ref.[2], using a rigorous definition of the Euclidean sum over histories. A proof using the configuration space propagator in the energy representation has also been given [4]. All of these proofs use the configuration space propagator, and the first two in particular, rely on the notion of sums over paths in configuration space. However, first crossing questions involving only position are clearly not the most general. It is reasonable to ask, for example, for the amplitude of a first crossing in momentum space.

In this paper, it is shown that the path decomposition expansion may be proved in a way that minimizes reliance on the properties of paths in configuration space. The proof uses projection operators rather than sums over histories. A form of the PDX is thus obtained which is valid for first crossings a wide class of observables, not just position. As an example, the PDX for the case of first crossing in momentum space is derived.

## 2. A NEW PROOF OF THE PATH DECOMPOSITION EXPANSION

Suppose configuration space is divided into two regions,  $C$ , and its complement  $\bar{C}$ , and let  $\Sigma$  be their common boundary. We are interested in the propagator from a point  $\mathbf{x}'$  in  $\bar{C}$  at  $t'$  to  $\mathbf{x}''$  in  $C$  at  $t''$ . Introduce the projection operator onto  $C$ ,

$$P_C = \int_C d^d \mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}| \quad (2.1)$$

Its complement  $P_{\bar{C}}$  is analogously defined, and we have the important relations,

$$P_C + P_{\bar{C}} = 1 \quad (2.2)$$

$$P_C P_{\bar{C}} = 0 \quad (2.3)$$

Introduce the discrete set of times  $t' = t_0 < t_1 < t_2 < \dots < t_n = t''$ . We will eventually take the continuum limit, in which  $(t_k - t_{k-1}) \rightarrow 0$ , and  $n \rightarrow \infty$ , whilst  $t_n - t_0$  remains constant. Introduce the Heisenberg picture projections

$$P(t) = e^{\frac{i}{\hbar}H(t-t_0)} P e^{-\frac{i}{\hbar}H(t-t_0)} \quad (2.4)$$

so  $P(t_0) = P$ .

The PDX follows directly from a resolution of the identity operator which we now derive. Consider the resolution of the identity (2.2) at time  $t_0$ . Multiplying the last term by the same resolution of the identity at time  $t_1$ , one obtains

$$1 = P_C(t_0) + P_C(t_1)P_{\bar{C}}(t_0) + P_{\bar{C}}(t_1)P_{\bar{C}}(t_0) \quad (2.5)$$

Multiplying the last term by the same resolution of the identity at  $t_2$ , and proceeding iteratively leads to the result

$$\begin{aligned} 1 = P_C(t_0) + \sum_{k=1}^n P_C(t_k)P_{\bar{C}}(t_{k-1}) \cdots P_{\bar{C}}(t_0) \\ + P_{\bar{C}}(t_n) \cdots P_{\bar{C}}(t_0) \end{aligned} \quad (2.6)$$

Each term in this sum corresponds to the statement that the particle is in  $\bar{C}$  at times  $t_0, t_1 \dots t_{k-1}$ , in  $C$  at  $t_k$ , and in  $\bar{C}$  or  $C$  at times  $t_{k+1}$  to  $t_n$ . In the continuum limit each term will therefore represent the statement that the particle crosses  $\Sigma$  for the first time at  $t_k$ . We cannot of course say this without taking the continuum limit, because the particle could be anywhere between each time at which the projection acts.

Now insert the resolution of the identity (2.6) into the expression for the propagator (1.1). Note first that we have

$$P_C(t_0)|\mathbf{x}'\rangle = 0 \quad (2.7)$$

since  $\mathbf{x}'$  is not in  $C$ , and

$$\langle \mathbf{x}'' | e^{-\frac{i}{\hbar}H(t_n-t_0)} P_{\bar{C}}(t_n) = 0 \quad (2.8)$$

since  $\mathbf{x}''$  is not in  $\bar{C}$ . It follows that

$$\langle \mathbf{x}'' | e^{-\frac{i}{\hbar}H(t_n-t_0)} |\mathbf{x}'\rangle = \sum_{k=1}^n \langle \mathbf{x}'' | e^{-\frac{i}{\hbar}H(t_n-t_0)} P_C(t_k)P_{\bar{C}}(t_{k-1}) \cdots P_{\bar{C}}(t_0) |\mathbf{x}'\rangle \quad (2.9)$$

since (2.7) and (2.8) imply that the first and last terms on the right-hand side of (2.6) do not contribute. When the time interval  $t_k - t_{k-1} = \delta t$  is small, we have

$$P_C(t_k) \approx P_C(t_{k-1}) + \delta t \dot{P}_C(t_{k-1}) + O(\delta t^2) \quad (2.10)$$

Using (2.3), it follows that

$$\begin{aligned} \langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t_n - t_0)} | \mathbf{x}' \rangle &= \sum_{k=1}^n \delta t \langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t_n - t_{k-1})} \dot{P}_C P_{\bar{C}} e^{-\frac{i}{\hbar} H(t_{k-1} - t_{k-2})} \\ &\quad \times P_{\bar{C}}(t_{k-2}) \cdots P_{\bar{C}}(t_0) | \mathbf{x}' \rangle \end{aligned} \quad (2.11)$$

This is now conveniently written,

$$\langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t_n - t_0)} | \mathbf{x}' \rangle = \sum_{k=1}^n \delta t \langle \phi | \dot{P}_C | \chi \rangle \quad (2.12)$$

where

$$\langle \phi | \mathbf{x} \rangle = \phi^*(\mathbf{x}) = \langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t_n - t_{k-1})} | \mathbf{x} \rangle \quad (2.13)$$

$$\langle \mathbf{x} | \chi \rangle = \chi(\mathbf{x}) = \langle \mathbf{x} | P_{\bar{C}} e^{-\frac{i}{\hbar} H(t_{k-1} - t_{k-2})} P_{\bar{C}}(t_{k-2}) \cdots P_{\bar{C}}(t_0) | \mathbf{x}' \rangle \quad (2.14)$$

Eq.(2.13) is clearly the propagator from  $(\mathbf{x}, t_{k-1})$  to  $(\mathbf{x}'', t_n)$ . In the continuum limit  $\delta t \rightarrow 0$ , Eq.(2.14) becomes the restricted propagator from  $\mathbf{x}'$  to  $\mathbf{x}$  in the region  $\bar{C}$ , and vanishes on the boundary  $\Sigma$  between  $C$  and  $\bar{C}$ .

This expression is readily simplified. Suppose the Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \quad (2.15)$$

Then

$$\dot{P}_C = \frac{i}{\hbar} [H, P_C] = \frac{i}{\hbar} \left[ \frac{\mathbf{p}^2}{2m}, P_C \right] \quad (2.16)$$

and it follows that

$$\begin{aligned} \langle \phi | \dot{P}_C | \chi \rangle &= \frac{i}{\hbar} \int_C d^d x \left( -\frac{\hbar^2}{2m} \chi \nabla^2 \phi^* + \frac{\hbar^2}{2m} \phi^* \nabla^2 \chi \right) \\ &= -\frac{i\hbar}{2m} \int_{\Sigma} d^{d-1} x \mathbf{n} \cdot (\chi \nabla \phi^* - \phi^* \nabla \chi) \end{aligned} \quad (2.17)$$

Now taking the continuum limit, the discrete sum becomes an integral, and  $\langle \mathbf{x} | \chi \rangle$  vanishes on  $\Sigma$ . Denoting  $t_k$  by  $t_\sigma$ , we thus obtain

$$\langle \mathbf{x}'' | e^{-\frac{i}{\hbar} H(t'' - t')} | \mathbf{x}' \rangle = \int_{t'}^{t''} dt_\sigma \int_{\Sigma} d^{d-1} \mathbf{x} \phi^*(\mathbf{x}) \frac{i\hbar}{2m} \mathbf{n} \cdot \nabla \chi(\mathbf{x}) \quad (2.18)$$

Inserting (2.13) and (2.14) yields the desired result, Eq.(1.4). If  $\mathbf{x}'$  and  $\mathbf{x}''$  are on the same side of  $\Sigma$ , in the region  $\bar{C}$  say, then the last term on the right-hand side of Eq.(2.6) also contributes, and the result (1.5) is obtained.

We have therefore derived the PDX in a way that appealed to the properties of the position operator only in the final steps, (2.16), (2.17). This points the way to a form of the PDX which should be valid for any projections onto any observable (provided the appropriate restricted propagators exist). In particular, the continuum limit of Eq.(2.6), multiplied by the unitary evolution operator yields

$$\begin{aligned} e^{-\frac{i}{\hbar}H(t''-t')} &= e^{-\frac{i}{\hbar}H(t''-t')} P_C \\ &+ \int_{t'}^{t''} dt_\sigma e^{-\frac{i}{\hbar}H(t''-t_\sigma)} \frac{i}{\hbar} [H, P_C] G^{(r)}(t_\sigma, t') \\ &+ G^{(r)}(t'', t') \end{aligned} \quad (2.19)$$

where

$$G^{(r)}(t_\sigma, t') = \lim e^{-\frac{i}{\hbar}H(t_\sigma-t')} P_{\bar{C}}(t_{k-1}) P_{\bar{C}}(t_{k-2}) \cdots P_{\bar{C}}(t_0) \quad (2.20)$$

and similarly for  $G^{(r)}(t'', t')$ , where the limit is  $\delta t \rightarrow 0$ ,  $k \rightarrow \infty$  with  $t_k - t_0$  held constant. Clearly the first term in (2.19) does not contribute for initial states with non-zero support in  $\bar{C}$  only. Eq.(2.19), a generalization of the PDX, is the main result of this paper.

### 3. FIRST CROSSING IN MOMENTUM SPACE

As an example of the generalized PDX, consider the case of first crossing in momentum space. For simplicity let the system be one-dimensional, and let the region  $C$  be  $p > 0$ , so  $\Sigma$  is the surface  $p = 0$ . Then

$$P_C = \int_0^\infty dp |p\rangle \langle p| \quad (3.1)$$

The PDX has the form

$$\langle p'' | e^{-\frac{i}{\hbar}H(t''-t')} | p' \rangle = \int_{t'}^{t''} dt_\sigma \langle \phi | \dot{P}_C | \chi \rangle \quad (3.2)$$

where

$$\langle \phi | p \rangle = \langle p'' | e^{-\frac{i}{\hbar}H(t''-t_\sigma)} | p \rangle = g(p'', t'' | p, t') \quad (3.3)$$

and

$$\langle p|\chi\rangle = g^{(r)}(p, t_\sigma|p', t') \quad (3.4)$$

Eq.(3.4) is the propagator in momentum space restricted to the region  $p < 0$  and vanishes on  $p = 0$ .

We have

$$\langle \phi|\dot{P}_C|\chi\rangle = \frac{i}{\hbar}\langle \phi|[V(x), P_C]|\chi\rangle \quad (3.5)$$

For simplicity, let  $V(x) = \frac{1}{2}m\omega^2 x^2$ . Then following steps closely analagous to those used in Eq.(2.17), it is readily seen that

$$\langle \phi|\dot{P}_C|\chi\rangle = -\frac{im\omega^2\hbar}{2}\left(\phi^*(p)\frac{\partial\chi(p)}{\partial p} - \frac{\partial\phi^*(p)}{\partial p}\chi(p)\right)_{p=0} \quad (3.6)$$

Since  $\chi(p)$  vanishes at  $p = 0$ , we derive the PDX in momentum space,

$$g(p'', t''|p', t') = -\frac{im\omega^2\hbar}{2}\int_{t'}^{t''} dt_\sigma g(p'', t''|p = 0, t_\sigma) \frac{\partial g^{(r)}}{\partial p}(p = 0, t_\sigma|p', t') \quad (3.7)$$

Other examples of the generalized PDX are easily constructed. Eq.(2.19) is valid for spin systems, for example, although it is less clear how useful it might be there. These and similar considerations will be pursued elsewhere.

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